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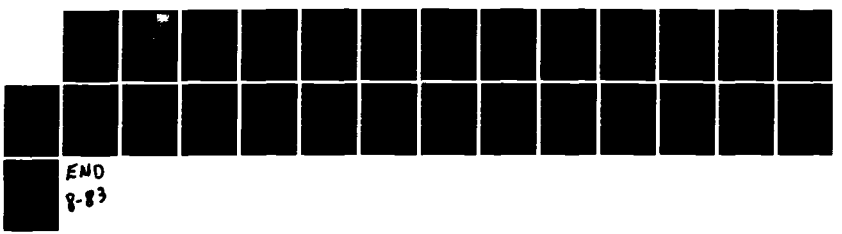

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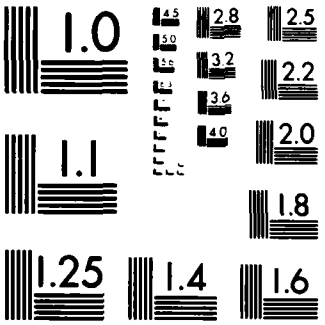

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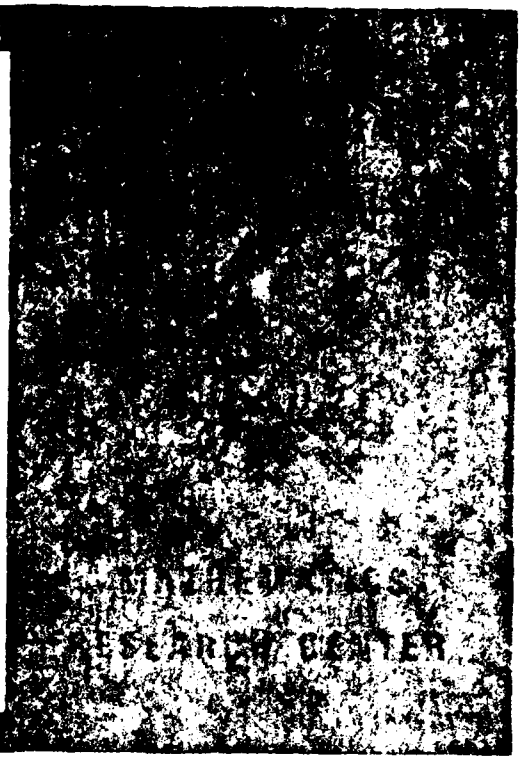
CONSTRAINED NONLINEAR LEAST SQUARES

George E. P. Box and Hiromitsu Kanemasu



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CONSTRAINED NONLINEAR LEAST SQUARES

George E. P. Box* and Hiromitsu Kanemasu**

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ABSTRACT

Gauss suggested that, when the model is a nonlinear function of parameters, least squares parameter estimates might be obtained by iterative linearization. To prevent difficulties in convergence, Levenberg, and later Marquardt, proposed a constrained minimization procedure using a scale-invariant metric for the parameters. If, as seems sensible, the minimization is conducted in a metric which is also linearly invariant then the Levenberg-Marquardt method is equivalent to a simple modification of the Gauss iteration proposed earlier. Methods for deciding, at each stage, how far to move along the Gauss solution vector are introduced which make economic use of the available information.

AMS (MOS) Subject Classification: 62J02

Key Words: Nonlinear least squares, Levenberg-Marquardt algorithm, Convergence

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SIGNIFICANCE AND EXPLANATION

The method of least squares is widely used for the fitting to data of functions containing unknown parameters. When these functions are non-linear in the parameters an iterative approach using successive local linearizations was suggested by Gauss. To encourage convergence various modifications and alternatives have been suggested. In particular (a) it has been proposed that, at the early stages, use of the method of steepest descent might speed convergence (b) a method might be used in which changes were made in the direction of, but not of the magnitude of, the Gauss adjustment. It is convenient to call this the Gauss direction method. (c) Levenberg and later Marquardt proposed a spherically constrained procedure. The procedure could be made scale-invariant to render its behavior independent of the (arbitrary) units in which the parameters were measured. It was argued the resulting method offered an appropriate compromise between steepest descent and Gauss's method.

In this report some of the geometry of these methods is discussed. As a consequence it is argued that the procedure should also be made invariant under linear transformation. With this modification (a) the scale-invariant Levenberg-Marquardt method becomes inappropriate and (b) the steepest descent direction and the Gauss direction become identical. It remains, therefore, to determine how far along the Gauss direction one should proceed. Two alternative methods for deciding this are suggested. Both methods use quantities already available from previous calculations.

CONSTRAINED NONLINEAR LEAST SQUARES

George E. P. Box* and Hiromitsu Kanemasu**

1. Nonlinear Least Squares

Suppose an observation y_u is described in the model

$$y_u = f(\underset{\sim}{\xi}_u, \underset{\sim}{\theta}) + \varepsilon_u, \qquad u = 1,2,\ldots,n \tag{1.1}$$

where $\underset{\sim}{\xi}_u = (\xi_{1u}, \xi_{2u}, \ldots, \xi_{ku})'$ are the levels of k independent variables, $\underset{\sim}{\theta} = (\theta_1, \theta_2, \ldots, \theta_p)'$ are p unknown parameters, $f(\underset{\sim}{\xi}_u, \underset{\sim}{\theta})$ is a known function of $\underset{\sim}{\xi}_u$ and $\underset{\sim}{\theta}$, and ε_u is a random error. The method of least squares obtains an estimate $\hat{\underset{\sim}{\theta}}$ of the parameters which minimizes the sum of squares

$$S(\underset{\sim}{\theta}) = \sum_{u=1}^{n} (y_u - f(\underset{\sim}{\xi}_u, \underset{\sim}{\theta}))^2 , \tag{1.2}$$

or in vector notation

$$S(\underset{\sim}{\theta}) = (\underset{\sim}{y} - \underset{\sim}{f}_{\underset{\sim}{\theta}})'(\underset{\sim}{y} - \underset{\sim}{f}_{\underset{\sim}{\theta}}) , \tag{1.3}$$

where $\underset{\sim}{y}$ is the $n \times 1$ vector of y_u, $u = 1,2,\ldots,n$ and $\underset{\sim}{f}_{\underset{\sim}{\theta}}$ is the $n \times 1$ vector whose u^{th} element is $f(\underset{\sim}{\xi}_u, \underset{\sim}{\theta})$. Under the assumption that the errors are independently and normally distributed with equal variance, $\hat{\underset{\sim}{\theta}}$ is the maximum likelihood estimator of $\underset{\sim}{\theta}$.

The function $f(\underset{\sim}{\xi}_u, \underset{\sim}{\theta})$ is said to be linear in the parameters if the derivatives $\partial f(\underset{\sim}{\xi}_u, \underset{\sim}{\theta})/\partial\theta_j$ are independent of $\underset{\sim}{\theta}$ for all j. Otherwise, it is called nonlinear. When the model is linear, the least squares estimates $\hat{\underset{\sim}{\theta}}$ are simply the solution of the normal equation $\underset{\sim}{X}'\underset{\sim}{X}\underset{\sim}{\theta} = \underset{\sim}{X}'\underset{\sim}{y}$ where $\underset{\sim}{X}$ is the $n \times p$ matrix of derivatives

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$\partial f(\underset{\sim}{\xi}_u,\underset{\sim}{\theta})/\partial\theta_j$. If the model is nonlinear Gauss [11] suggested that $\hat{\underset{\sim}{\theta}}$ could be obtained by linearizing $f(\underset{\sim}{\xi}_u,\underset{\sim}{\theta})$ around the current estimates $\underset{\sim}{\theta}^{(o)}$ in successive iterations.

2. Gauss Method and Overshooting

A local approximation to the nonlinear function $f(\underset{\sim}{\xi}_u,\underset{\sim}{\theta})$ may be obtained by performing a Taylor series expansion at some guessed values $\underset{\sim}{\theta} = \underset{\sim}{\theta}^{(o)}$, and truncating after first order terms to obtain

$$f(\underset{\sim}{\xi}_u,\underset{\sim}{\theta}) \cong f(\underset{\sim}{\xi}_u,\underset{\sim}{\theta}^{(o)}) + \sum_{i=1}^{p} \left[\frac{\partial f(\underset{\sim}{\xi}_u,\underset{\sim}{\theta})}{\partial\theta_i}\right]_{\underset{\sim}{\theta}=\underset{\sim}{\theta}^{(o)}} (\theta_i - \theta_i^{(o)}) \quad u = 1,2,\ldots, n \ . \tag{2.1}$$

In vector notation

$$\underset{\sim}{f}_{\underset{\sim}{\theta}} \cong \underset{\sim}{f}_o + \underset{\sim}{X}_o(\underset{\sim}{\theta} - \underset{\sim}{\theta}^{(o)}) \ , \tag{2.2}$$

where $\underset{\sim}{f}_o$ is the $n \times 1$ vector of $f(\underset{\sim}{\xi}_u,\underset{\sim}{\theta}^{(o)})$; $u = 1,2,\ldots,n$ and $\underset{\sim}{X}_o$ is the $n \times p$ matrix whose (u,j) element is $[\partial f(\underset{\sim}{\xi}_u,\underset{\sim}{\theta})/\partial\theta_j]_{\underset{\sim}{\theta}=\underset{\sim}{\theta}^{(o)}}$. This local linearization gives the approximate sum of squares

$$\bar{S}(\underset{\sim}{\theta}) = (\underset{\sim}{y} - \underset{\sim}{f}_o - \underset{\sim}{X}_o(\underset{\sim}{\theta} - \underset{\sim}{\theta}^{(o)}))'(\underset{\sim}{y} - \underset{\sim}{f}_o - \underset{\sim}{X}_o(\underset{\sim}{\theta} - \underset{\sim}{\theta}^{(o)}))$$

$$= \underset{\sim}{\varepsilon}_o'\underset{\sim}{\varepsilon}_o - 2\underset{\sim}{\varepsilon}_o'\underset{\sim}{X}_o(\underset{\sim}{\theta} - \underset{\sim}{\theta}^{(o)}) + (\underset{\sim}{\theta} - \underset{\sim}{\theta}^{(o)})'\underset{\sim}{X}_o'\underset{\sim}{X}_o(\underset{\sim}{\theta} - \underset{\sim}{\theta}^{(o)}) \tag{2.3}$$

where $\underset{\sim}{\varepsilon}_o = \underset{\sim}{y} - \underset{\sim}{f}_o$. Setting the derivatives $\partial\bar{S}(\underset{\sim}{\theta})/\partial\theta_j$ to zero gives the normal equations

$$\underset{\sim}{X}_o'\underset{\sim}{X}_o(\underset{\sim}{\theta} - \underset{\sim}{\theta}^{(o)}) = \underset{\sim}{X}_o'\underset{\sim}{\varepsilon}_o \ . \tag{2.4}$$

Thus provided that $X_o'X_o$ is nonsingular, new estimates $\underset{\sim}{\theta}^{(1)}$ of the parameters are given by

$$\underset{\sim}{\theta}^{(1)} - \underset{\sim}{\theta}^{(o)} = (\underset{\sim}{X}_o'\underset{\sim}{X}_o)^{-1}\underset{\sim}{X}_o'\underset{\sim}{\varepsilon}_o \ . \tag{2.5}$$

By linearizing now about $\underset{\sim}{\theta}^{(1)}$, a second approximation $\underset{\sim}{\theta}^{(2)}$ may now be obtained, and so on. Figure 1 shows the parameter space representation of the first stage of this procedure for a two parameter model. Contours for true and approximate sums of squares $S(\underset{\sim}{\theta})$ and $\bar{S}(\underset{\sim}{\theta})$ are shown. Contours of $\bar{S}(\underset{\sim}{\theta})$ are necessarily elliptical while those for $S(\underset{\sim}{\theta})$ have the appearance of distorted ellipses.

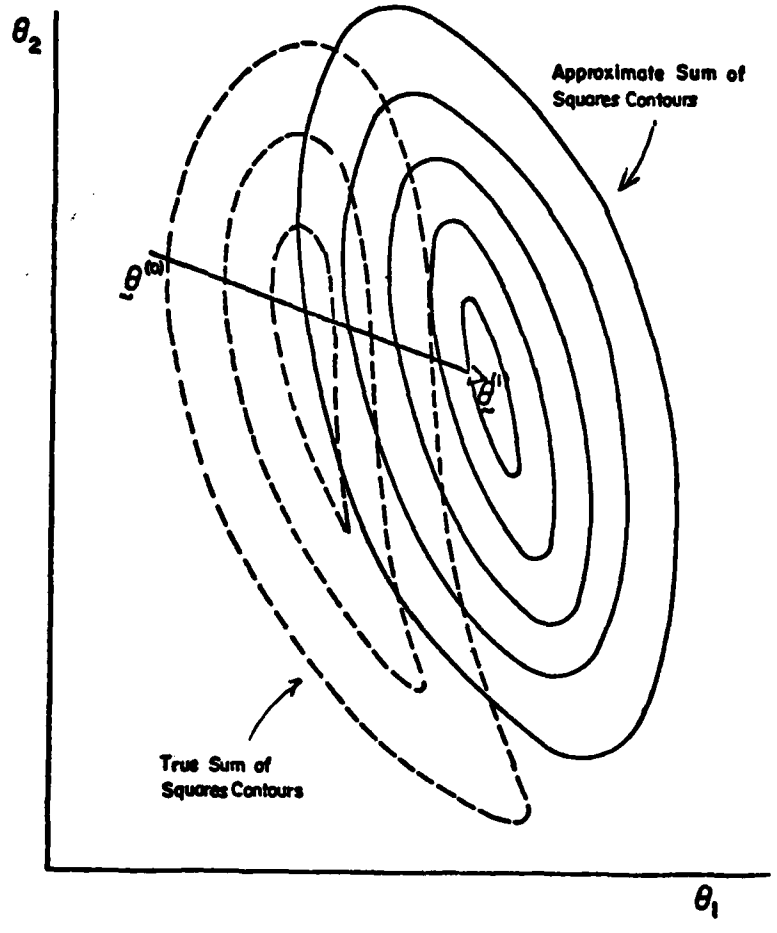

Figure 1. Parameter space representation of the Gauss iteration.

In favorable circumstances the iteration will converge to the least squares estimates but in some examples wild oscillations can occur from one iteration to another and the process may not converge. Figure 1 shows a typical case of initial divergence, where the Gauss solution vector (2.5) "overshoots" and the true sum of squares given by the new estimates $\underset{\sim}{\theta}^{(1)}$ is larger than that given by the initial estimates $\underset{\sim}{\theta}^{(o)}$. A frequent cause of divergence is that the adjustment $\underset{\sim}{\theta}^{(1)} - \underset{\sim}{\theta}^{(o)}$ is too large and so invalidates the linear approximation (2.1).

3. Steepest Descent Approach and Application of Response Surface Method

Another iterative approach to nonlinear least squares uses steepest descent where initially the iteration moves from the current point $\underset{\sim}{\theta}^{(o)}$ in the direction of steepest descent vector, that is $-\left(\frac{\partial S(\underset{\sim}{\theta})}{\partial \theta_1}, \ldots, \frac{\partial S(\underset{\sim}{\theta})}{\partial \theta_p}\right)'$ evaluated at $\underset{\sim}{\theta} = \underset{\sim}{\theta}^{(o)}$. This procedure is often effective in getting near the region of a minimum quickly. However, it may have an extremely slow rate of convergence after that, particularly in the common case of a ridgy minimum.

Box and Coutie [6] proposed a method based on response surface methodology which employed steepest descent at the early stages [2],[9]. If the initial point is remote from the minimum, the sum of squares surface $S(\underset{\sim}{\theta})$ might be capable of local approximation by a polynomial in $\underset{\sim}{\theta}$ of the first degree. The sum of squares is therefore determined at a series of points in the parameter space from which a planar approximation may be fitted and the direction of steepest descent calculated. This direction is followed until an increase in the sum of squares is encountered. The whole process is repeated until the need for a second degree approximation becomes manifest.

Sums of squares are then computed at a set of points arranged to allow a second degree polynomial to be locally fitted, and an approximate minimum determined. This method is (see also Koshal [13]) inefficient because it makes use of only the information contained in the sum of squares of residuals but not of that in the individual

residuals themselves. It was shown in [3] that when this missing information is included we are brought back to the Gauss method.

4. Modified Gauss Iteration

One way to overcome the difficulty of overshooting in the Gauss iteration is to determine direction only (but not distance) by the Gauss solution vector $\underset{\sim}{\theta}^{(g)} - \underset{\sim}{\theta}^{(o)} = (\underset{\sim o}{X'}\underset{o}{X})^{-1}\underset{o}{X'}\underset{o}{\varepsilon}$. Thus, the adjustment vector $\underset{\sim}{\theta} - \underset{\sim}{\theta}^{(o)}$ is given by

$$\underset{\sim}{\theta} - \underset{\sim}{\theta}^{(o)} = v(\underset{\sim o}{X'}\underset{o}{X})^{-1}\underset{o}{X'}\underset{o}{\varepsilon} \tag{4.1}$$

where v is a positive quantity usually less than unity. This modified Gauss iteration was suggested by Box [4] and incorporated into a computer program described by Booth, Box, Muller and Peterson [1]. In order to determine the value of v that approximately minimizes the sum of squares along the Gauss solution vector, they used the "halving and doubling" method in which, starting from $v = 1$, the value of v is successively halved (or doubled) until the sum of squares finally starts to increase and then a quadratic curve is fitted to the last three points to locate an approximate local minimum. Hartley [12] later proved that, under a set of mild regularity conditions, the modified Gauss iteration as described above converges to the solution of $\partial S(\underset{\sim}{\theta})/\partial\theta_j = 0;\ j = 1,2,\ldots,p$ and also proposed a similar method to determine the value of v.

5. Levenberg-Marquardt's Constrained Iteration

5.1. Levenberg's Damped Least Squares

Levenberg [14] tried to overcome the difficulty of "overshooting" in the Gauss iteration by introducing a constraint into the minimization of the sum of squares. Instead of minimizing the approximate sum of squares $\bar{S}(\underset{\sim}{\theta})$ itself he proposed to minimize

$$F(\underset{\sim}{\theta}) = \bar{S}(\underset{\sim}{\theta}) + \lambda \sum_{i=1}^{p} \omega_i(\theta_i - \theta_i^{(o)})^2 \tag{5.1}$$

where $\lambda\omega_1, \lambda\omega_2, \ldots, \lambda\omega_p$ are positive weighting factors expressing the relative importance

of damping the different increments. Substituting (2.3) into (5.1),

$$F(\underset{\sim}{\theta}) = \underset{\sim o}{\varepsilon}'\underset{\sim o}{\varepsilon} - 2\underset{\sim o}{\varepsilon}'\underset{o\,o}{X}(\underset{\sim}{\theta} - \underset{\sim}{\theta}^{(o)}) + (\underset{\sim}{\theta} - \underset{\sim}{\theta}^{(o)})'\underset{o\,o}{X'X}(\underset{\sim}{\theta} - \underset{\sim}{\theta}^{(o)})$$

$$+ \lambda(\underset{\sim}{\theta} - \underset{\sim}{\theta}^{(o)})'\Omega(\underset{\sim}{\theta} - \underset{\sim}{\theta}^{(o)}) \ , \tag{5.2}$$

where Ω is a $p \times p$ diagonal matrix whose i^{th} diagonal element is ω_i. Setting the derivatives $\partial F(\underset{\sim}{\theta})/\partial\theta_i$ to zero

$$-\underset{o\,o}{X'}\underset{\sim o}{\varepsilon} + \underset{o\,o}{X'X}(\underset{\sim}{\theta} - \underset{\sim}{\theta}^{(o)}) + \lambda\Omega(\underset{\sim}{\theta} - \underset{\sim}{\theta}^{(o)}) = \underset{\sim}{0} \ . \tag{5.3}$$

Solving for $\underset{\sim}{\theta}$, we have

$$\underset{\sim}{\theta} - \underset{\sim}{\theta}^{(o)} = (\underset{\sim o\,o}{X'X} + \lambda\Omega)^{-1}\underset{\sim o\,o}{X'}\underset{\sim o}{\varepsilon} \ . \tag{5.4}$$

Geometrically, in the parameter space representation, this amounts to minimizing the approximate sum of squares $\bar{S}(\underset{\sim}{\theta})$ on the elliptical constraint whose principal axes are parallel to the axes of $\theta_1,\theta_2,\ldots,\theta_p$. This is illustrated in Figure 2. The dotted curve represents the locus of the solution of (5.4) for various values of λ. Levenberg proved that, provided the true sum of squares $S(\underset{\sim}{\theta})$ does not already have a stationary value at the current estimate $\underset{\sim}{\theta}^{(o)}$, the sum of squares initially decreases as we move off the point $\underset{\sim}{\theta}^{(o)}$. He recommended the spherical constraint $\underset{\sim}{\Omega} = \underset{\sim p}{I}$, where $\underset{\sim p}{I}$ is the $p \times p$ identity matrix. An alternative choice for $\underset{\sim}{\Omega}$ was a diagonal matrix $\underset{\sim}{D}$ whose j^{th} diagonal element was the j^{th} diagonal element $[jj]$ of the matrix $\underset{\sim o\,o}{X'X}$.

5.2. Marquardt's Algorithm

Marquardt [15], also considered the constrained minimization. He examined geometrical aspects of the case $\underset{\sim}{\Omega} = \underset{\sim p}{I}$ in Levenberg's formulation. He noted a result of Morrison [17] that the radius of the constraining sphere is a monotone decreasing function of λ that tends to zero as $\lambda \to \infty$, and then proved that as $\lambda \to \infty$ the solution vector of the constrained minimization rotates toward the steepest descent vector that remains fixed. Since the Gauss solution is of course a special case of the constrained minimization when $\lambda = 0$, a choice of some intermediate value for λ would provide a compromise between the two classical methods. The algorithm proposed by Marquardt, which

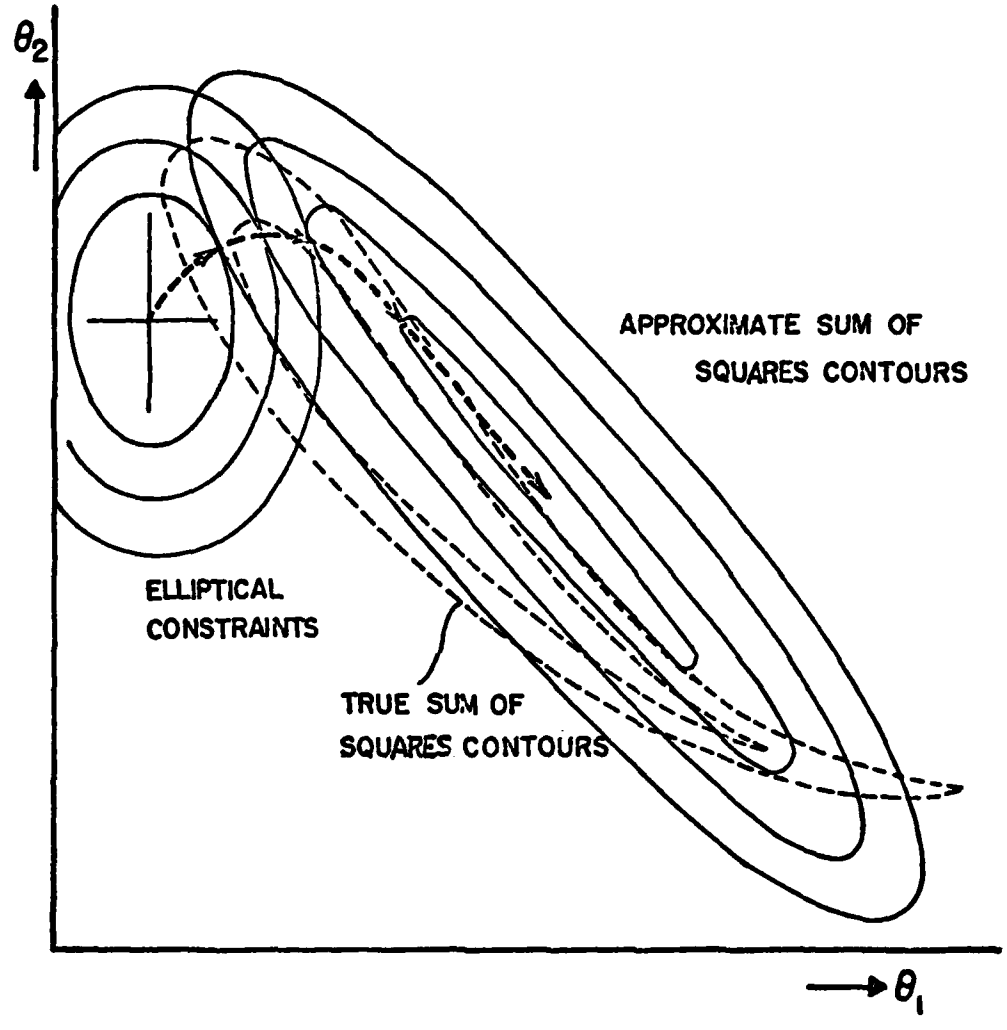

Figure 2. Parameter space representation of Levenberg's constrained minimization.

may be termed (λ,ν) algorithm, reduces the level of λ by a factor ν from a relatively large initial value λ_o as the iteration proceeds. This amounts to making use of the steepest descent-like procedure early in the iterative process and then later shifting to a solution that approximates the Gauss solution. Marquardt's method thus appears to possess the virtue of using each classical procedure in the circumstances where it is most effective.

Noting that the steepest descent procedure is dependent on the choice of parameter scales, Marquardt proposed the constrained minimization in the scale invariant metric, i.e., the minimization with a spherical constraint in $\theta_j^* = [jj]^{1/2}\theta_j$ $(j = 1,2,\ldots,p)$. This is equivalent to using the constraint $\underset{\sim}{\Omega} = \underset{\sim}{D}$ of Levenberg. Marquardt's recommendations were followed by Meeter [16] in the program GAUSHAUS at the University of Wisconsin and similar programs have been used elsewhere.

5.3. Constrained Minimization in the Transformed Space

The Levenberg-Marquardt procedure may be criticized as follows. The use of constant spherical or elliptical constraints implies that it is logical to solve the problem in some parameterization decided in advance by the investigator. However, usually there are many ways in which a problem might be parameterized. Instead of considering $\theta_1,\theta_2,\ldots,\theta_p$, we might with equal reason consider $\psi_1,\psi_2,\ldots,\psi_p$ where $\psi_j = \psi_j(\underset{\sim}{\theta})$ is some 1:1 transformation of $\underset{\sim}{\theta}$. Clearly, the nature of the constraints applied would differ depending on which parameterization was adopted.

Let us then consider the problem in a parameter metric that is not only scale invariant but also invariant under <u>linear transformation</u>. Such parameter metric $\underset{\sim}{\psi}$ is provided by $\underset{\sim}{\psi} = \underset{\sim}{H}\underset{\sim}{\theta}$ where $\underset{\sim}{H}$ is any $p \times p$ nonsingular matrix that satisfies

$$\underset{\sim}{H}'\underset{\sim}{H} = \underset{\sim}{X}_o'\underset{\sim}{X}_o \,. \tag{5.5}$$

To see this, make an arbitrary linear transformation $\bar{\underset{\sim}{\theta}} = \underset{\sim}{L}\underset{\sim}{\theta}$. Correspondingly the derivative matrix X_o will be transformed to $\bar{X}_o = X_o L^{-1}$. The transformation of $\bar{\underset{\sim}{\theta}}$ corresponding to $\underset{\sim}{\theta} \to \underset{\sim}{\psi}$ will be $\bar{\underset{\sim}{\psi}} = \bar{\underset{\sim}{H}}\bar{\underset{\sim}{\theta}}$ with $\bar{H}'\bar{H} = \bar{X}_o'\bar{X}_o$. However, the requirement on

$\bar{H}$ will be satisfied by $\bar{H} = HL^{-1}$ since

$$\bar{H}'\bar{H} = (HL^{-1})'(HL^{-1}) = L^{-1'}X_o'X_oL^{-1} = \bar{X}_o'\bar{X}_o \ . \tag{5.6}$$

Therefore

$$\underset{\sim}{\bar{\psi}} = \bar{H}\bar{\theta} = (HL^{-1})(L\underset{\sim}{\theta}) = H\underset{\sim}{\theta} = \underset{\sim}{\psi} \ , \tag{5.7}$$

establishing that $\underset{\sim}{\psi}$ is invariant under linear transformation.

In the new space $\underset{\sim}{\psi}$ the linearized model will be

$$\underset{\sim}{f}_{\psi} \cong \underset{\sim}{f}_o + Z_o(\underset{\sim}{\psi} - \underset{\sim}{\psi}^{(o)}) \tag{5.8}$$

where $\underset{\sim}{f}_{\psi}$ is the $n \times 1$ vector of $f(\underset{\sim}{\xi}_u, \underset{\sim}{\theta}(\underset{\sim}{\psi}))$; $u = 1,2,\ldots,n$, $\underset{\sim}{\psi}^{(o)} = H\underset{\sim}{\theta}^{(o)}$, and Z_o is the $n \times p$ matrix whose (u,j) element is $[\partial f(\underset{\sim}{\xi}_u, \underset{\sim}{\theta}(\underset{\sim}{\psi}))/\partial\psi_j]_{\underset{\sim}{\psi}=\underset{\sim}{\psi}^{(o)}}$. Notice that Z_o is related to X_o by $Z_o = X_oH^{-1}$. Therefore, the sum of squares contours for the linearized model given by

$$(\underset{\sim}{y} - \underset{\sim}{f}_o - Z_o(\underset{\sim}{\psi} - \underset{\sim}{\psi}^{(o)}))'(\underset{\sim}{y} - \underset{\sim}{f}_o - Z_o(\underset{\sim}{\psi} - \underset{\sim}{\psi}^{(o)})) = \text{constant} \tag{5.9}$$

will be spherical because

$$Z_o'Z_o = (X_oH^{-1})'(X_oH^{-1}) = H^{-1'}X_o'X_oH^{-1} = I_p \ . \tag{5.10}$$

The representation of the problem would now be that illustrated for $p = 2$ in Figure 3 in which the contours for the linearized model are spheres. To the extent that the contours for the linearized model were like those for the true model, this would ensure that the contours of the true model were roughly spherical, enabling us to circumvent the difficulties arising in situations of ridgy minimum.

If, in the linearly invariant metric, we apply appropriate spherical constraints we must minimize

$$\begin{aligned} F(\underset{\sim}{\psi}) = {} & [\underset{\sim}{\varepsilon}_o - Z_o(\underset{\sim}{\psi} - \underset{\sim}{\psi}^{(o)})]'[\underset{\sim}{\varepsilon}_o - Z_o(\underset{\sim}{\psi} - \underset{\sim}{\psi}^{(o)})] \\ & + \lambda[(\underset{\sim}{\psi} - \underset{\sim}{\psi}^{(o)})'(\underset{\sim}{\psi} - \underset{\sim}{\psi}^{(o)}) - \gamma^2] \ , \end{aligned} \tag{5.11}$$

where $\underset{\sim}{\varepsilon}_o = \underset{\sim}{y} - \underset{\sim}{f}_o$ and γ is the radius of the sphere. Setting the derivatives $\partial F(\underset{\sim}{\psi})/\partial\psi_i$ $(i = 1,\ldots,p)$ to zero,

$$-2Z_o'\underset{\sim}{\varepsilon}_o + 2Z_o'Z_o(\underset{\sim}{\psi} - \underset{\sim}{\psi}^{(o)}) + 2\lambda(\underset{\sim}{\psi} - \underset{\sim}{\psi}^{(o)}) = 0 \ . \tag{5.12}$$

Solving for $\underset{\sim}{\psi}$ we obtain

$$\underset{\sim}{\psi} - \underset{\sim}{\psi}^{(o)} = (Z_o'Z_o + \lambda I_p)^{-1}Z_o'\underset{\sim}{\varepsilon}_o \ . \tag{5.13}$$

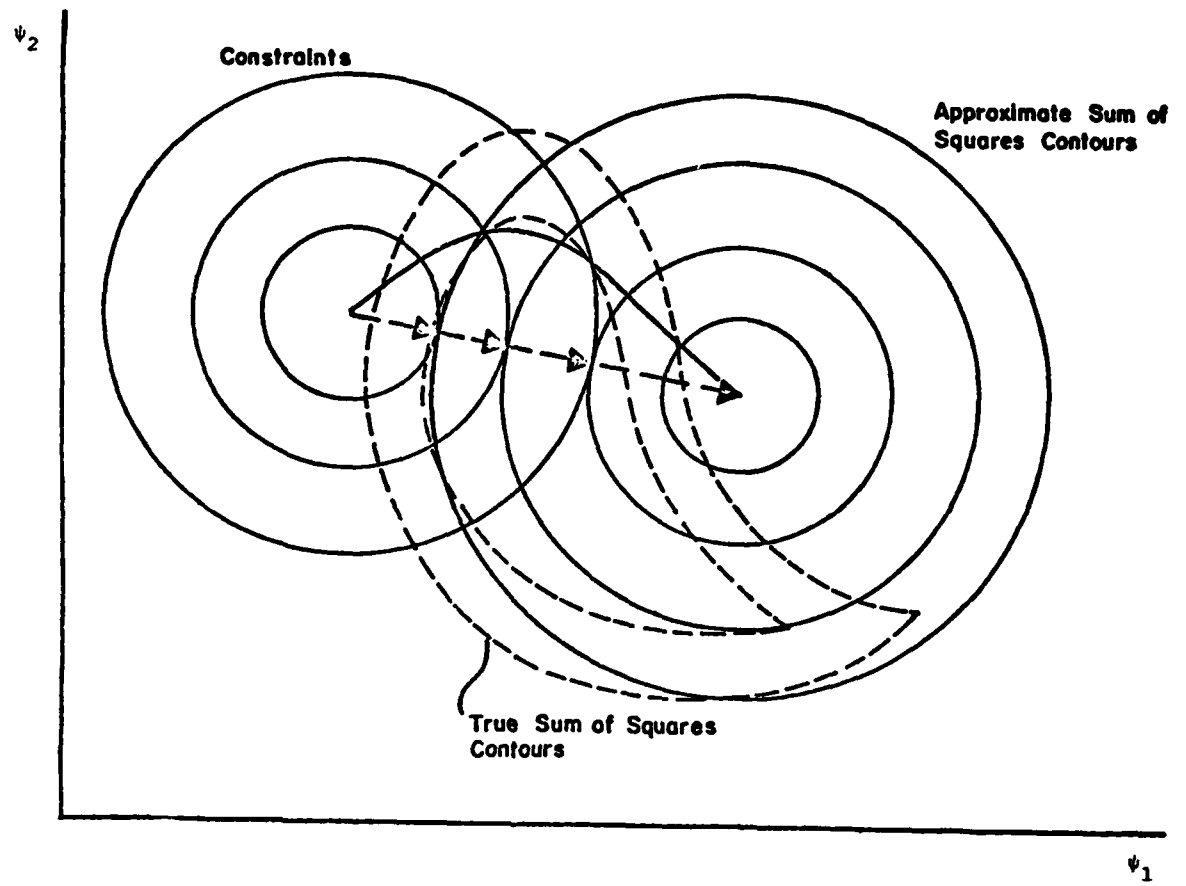

Figure 3. Constrained minimization of the sum of squares in the linearly invariant metric.

Because of (5.10), this is

$$\underset{\sim}{\psi} - \underset{\sim}{\psi}^{(o)} = \frac{1}{1 + \lambda} \underset{\sim o \sim o}{Z'\varepsilon} \quad . \tag{5.14}$$

It can be shown that, as long as $(-\lambda)$ is chosen to be less than the minimum eigenvalue of $Z_o'Z_o$ (that is, less than unity), the solution (5.13) provides the point that minimizes in the space $\underset{\sim}{\psi}$ the linearized model sum of squares on the sphere of radius $(1/1 + \lambda)^2 \underset{\sim o}{\varepsilon'} Z_o Z' \underset{\sim o \sim o}{\varepsilon}$. (See Draper [10] for the analysis of stationary points of the general quadratic response surface on spherical constraints.) We also note that this solution is the vector of steepest descent (except for the irrelevant scalar) since by differentiating the negative of the true sum of squares $S(\underset{\sim}{\psi}) = (\underset{\sim}{y} - \underset{\sim \underset{\sim}{\psi}}{f})'(\underset{\sim}{y} - \underset{\sim \underset{\sim}{\psi}}{f})$ with $\underset{\sim}{\psi}$ and evaluating the derivative at $\underset{\sim}{\psi} = \underset{\sim}{\psi}^{(o)}$ we obtain $2\underset{\sim o \sim o}{Z'\varepsilon}$. Now transforming (5.14) back to the original metric $\underset{\sim}{\theta}$,

$$H(\underset{\sim}{\theta} - \underset{\sim}{\theta}^{(o)}) = \frac{1}{1 + \lambda} (\underset{\sim o \sim}{X} H^{-1})' \underset{\sim o}{\varepsilon} \quad , \tag{5.15}$$

which gives

$$\underset{\sim}{\theta} - \underset{\sim}{\theta}^{(o)} = \frac{1}{1 + \lambda} H^{-1} (X_o H^{-1})' \underset{\sim o}{\varepsilon} = \frac{1}{1 + \lambda} (H'H)^{-1} \underset{o \sim o}{X'\varepsilon} \quad . \tag{5.16}$$

Because of (5.5), we finally obtain

$$\underset{\sim}{\theta} - \underset{\sim}{\theta}^{(o)} = \frac{1}{1 + \lambda} (X_o'X_o)^{-1} \underset{o \sim o}{X'\varepsilon} \quad . \tag{5.17}$$

This is the same as (4.1), where the requirement $(-\lambda) < 1$ implies that $v = 1/(1 + \lambda)$ can range between 0 and ∞. Somewhat surprisingly then the Levenberg-Marquardt constrained minimization performed in the linearly invariant metric is exactly the modified Gauss method discussed earlier. It should be noted also that in the linearly invariant metric there is no question of a compromise between the two classical methods. Because, using (5.10), the Gauss vector $(\underset{\sim o \sim o}{Z'Z})^{-1} \underset{\sim o \sim o}{Z'\varepsilon}$ is equal to $\underset{\sim o \sim o}{Z'\varepsilon}$ which is the steepest descent vector. (In Figure 3, the path that is the Gauss vector as well as the steepest descent vector is shown by the dotted straight line. The path which the Levenberg-Marquardt procedure would take is shown by the bold connected curve.)

So far as the problem of speedy convergence is concerned, there does not therefore seem to exist much concrete theoretical basis for interpolation between the two classical methods. One incidental advantage of the Levenberg-Marquardt procedure may be that the

matrix $(X'_{o}X_{o} + \lambda\Omega)$ can be inverted even when the matrix $X'_{o}X_{o}$ is singular or nearly singular, thus always giving a "solution". Practical experience, however, leads us to believe that the possibility of not having a singularity or near-singularity brought to one's attention is a disadvantage rather than an advantage. It has often been pointed out (for example [2]) that a minimum is often better approximated by a line, plane, or hyperplane than by a point. When this happens, it is important that it be brought to the investigator's notice. One method for ensuring this is by means of canonical analysis suggested, for example, in [5].

6. Methods to Determine How Far One Should Go Along the Gauss Solution Vector

In the preceding section, we have given theoretical support to the idea that we should explore the Gauss vector itself rather than the path followed by the Levenberg-Marquardt procedure. We have done this by demonstrating that the Gauss vector may be arrived at by applying Levenberg-Marquardt constrained minimization in the linearly invariant parameter metric.

We recall that the direction of the Gauss vector in the original parameter metric corresponds to that of the steepest descent considered in the linearly invariant metric. Also applying the Levenberg's result mentioned in Section 5.1 to the constrained minimization in the linearly invariant metric, we can be assured that the true sum of squares initially decreases as we start off from the current estimate $\theta^{(o)}$ on the Gauss vector provided $\theta^{(o)}$ is not already the stationary point.

The question of how far one should go along the Gauss vector still remains. The "halving and doubling" method already mentioned could be used. But its disadvantage is that, after the Gauss vector is determined for $\theta^{(o)}$, the function $f(\xi_u,\theta)$ must be additionally evaluated for $u = 1,2,\ldots,n$ to calculate $S(\theta)$ at each new "test point" in the parameter space. We also could apply the (λ,ν) algorithm of Marquardt to (5.17). Although no compromise between the original Gauss method and the steepest descent method is here involved, it may still make sense to gradually decrease λ so as to constrain the

iteration less and less as the minimum is approached in successive iterations. Again, however, there is no way to know in advance how best to choose λ_o and ν. Below we present two methods to determine the value of ν in (4.1) at each iteration in such a way as to make use of only the information already available from the preceding computation.

Modification A. To obtain the Gauss solution vector it is necessary to compute the matrix X_o of the partial derivatives $[\partial f(\underset{\sim}{\xi}_u, \underset{\sim}{\theta})/\partial\theta_j]_{\theta=\theta^{(o)}}$. Using this matrix, it is clearly possible to obtain the initial rate of change of the true sum of squares along the Gauss solution vector. In fact,

$$\left[\frac{dS}{d\nu}\right]_{\nu=0} = \sum_{i=1}^{p} \left[\frac{\partial S}{\partial \theta_i}\right]_{\nu=0} \left[\frac{d\theta_i}{d\nu}\right]_{\nu=0} = \left[\frac{\partial S}{\partial \underset{\sim}{\theta}}\right]'_{\nu=0} \left[\frac{d\underset{\sim}{\theta}}{d\nu}\right]_{\nu=0} \tag{6.1}$$

where $\left[\frac{\partial S}{\partial \underset{\sim}{\theta}}\right]_{\nu=0}$ is the $p \times 1$ vector of $\left[\frac{\partial S}{\partial \theta_i}\right]_{\nu=0}$; $i = 1,2,\ldots,p$, and $\left[\frac{d\underset{\sim}{\theta}}{d\nu}\right]_{\nu=0}$ is the $p \times 1$ vector of $\left[\frac{d\theta_i}{d\nu}\right]_{\nu=0}$; $i = 1,2,\ldots,p$. However, since $S = (\underset{\sim}{y} - \underset{\sim}{f}_\theta)'(\underset{\sim}{y} - \underset{\sim}{f}_\theta)$ and $\underset{\sim}{\theta} - \underset{\sim}{\theta}^{(o)} = \nu(X'_o X_o)^{-1} X'_o \underset{\sim}{\varepsilon}_o$, we obtain

$$\left[\frac{dS}{d\nu}\right]_{\nu=0} = -2\underset{\sim}{\varepsilon}'_o X_o (X'_o X_o)^{-1} X'_o \underset{\sim}{\varepsilon}_o = -2(\underset{\sim}{\theta}^{(g)} - \underset{\sim}{\theta}^{(o)})' X'_o \underset{\sim}{\varepsilon}_o . \tag{6.2}$$

Incidentally, equation (6.2) gives a direct proof of a corollary of Levenberg's result mentioned above that the true sum of squares initially decreases as we start moving from $\underset{\sim}{\theta}^{(o)}$ to $\underset{\sim}{\theta}^{(g)}$, because provided that $X'_o X_o$ is positive definite $\left[\frac{dS}{d\nu}\right]_{\nu=0}$ will be negative except when $X'_o \underset{\sim}{\varepsilon}_o = -\frac{1}{2}\left[\frac{\partial S}{\partial \underset{\sim}{\theta}}\right]_{\nu=0}$ is $\underset{\sim}{0}$.

To locate a point along the Gauss solution vector at which the true sum of squares is approximately minimized, we first suppose that the true sum of squares follows, along this vector, a quadratic function $S = a + b\nu + c\nu^2$. We can determine the constants a, b and c by setting $S = S_o$ for $\nu = 0$, $S = S_g$ for $\nu = 1$ and setting $\left[\frac{dS}{d\nu}\right]_{\nu=0}$ to that given by (6.2). Consequently, provided $c = S_g - S_o + 2(\underset{\sim}{\theta}^{(g)} - \underset{\sim}{\theta}^{(o)})' X'_o \underset{\sim}{\varepsilon}_o > 0$, the

value of v for which the true sum of squares is approximately minimized is given by

$$v_{min} = \frac{(\underset{\sim}{\theta}^{(g)} - \underset{\sim}{\theta}^{(o)})'X'_{o}\underset{\sim}{\varepsilon}_{o}}{S_g - S_o + 2(\underset{\sim}{\theta}^{(g)} - \underset{\sim}{\theta}^{(o)})'X'_{o}\underset{\sim}{\varepsilon}_{o}} . \tag{6.3}$$

Thus, we may take our next estimate as $\underset{\sim}{\theta}^{(1)} = \underset{\sim}{\theta}^{(o)} + v_{min}(\underset{\sim}{\theta}^{(g)} - \underset{\sim}{\theta}^{(o)})$. If $c < 0$, we have that the actual sum of squares S_g at distance $v = 1$ is already smaller than that predicted by the initial slope since in this case $S_g < S_o + [dS/dv]_{v=0}$. Therefore we may settle at $v = 1$, or double, or redouble the distance, checking at each point to see if the decreasing trend is continuing. Figure 4 illustrates various situations that could occur.

Modification B. A procedure developed following a suggestion by Jack Draffen[1] is another method that makes use of the existing information in an interesting manner. The quantities S_o and S_g are obtained by computing, squaring, and summing the elements of the two residual vectors

$$\underset{\sim}{\varepsilon}'_{o} = (y_1 - f(\underset{\sim}{\xi}_1,\underset{\sim}{\theta}^{(o)}), y_2 - f(\underset{\sim}{\xi}_2,\underset{\sim}{\theta}^{(o)}), \ldots, y_n - f(\underset{\sim}{\xi}_n,\underset{\sim}{\theta}^{(o)}))$$

and

$$\underset{\sim}{\varepsilon}'_{g} = (y_1 - f(\underset{\sim}{\xi}_1,\underset{\sim}{\theta}^{(g)}), y_2 - f(\underset{\sim}{\xi}_2,\underset{\sim}{\theta}^{(g)}), \ldots, y_n - f(\underset{\sim}{\xi}_n,\underset{\sim}{\theta}^{(g)})) . \tag{6.4}$$

Consider a point along the Gauss solution vector with the distance $v\|\underset{\sim}{\theta}^{(g)} - \underset{\sim}{\theta}^{(o)}\|$ away from the origin $\underset{\sim}{\theta}^{(o)}$. By linear interpolation we can estimate the residuals at this point by

$$\underset{\sim}{\varepsilon} = (1 - v)\underset{\sim}{\varepsilon}_{o} + v\underset{\sim}{\varepsilon}_{g} \tag{6.5}$$

which may be written

$$\underset{\sim}{\varepsilon}_{o} = v(\underset{\sim}{\varepsilon}_{o} - \underset{\sim}{\varepsilon}_{g}) + \underset{\sim}{\varepsilon} . \tag{6.6}$$

Thus the value $\hat{v}$ of v for which the sum of squares of the estimated residuals will be as small as possible can be obtained by regressing $\underset{\sim}{\varepsilon}_{o}$ on $\underset{\sim}{\varepsilon}_{o} - \underset{\sim}{\varepsilon}_{g}$ so that

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[1]Personal communication (1972).

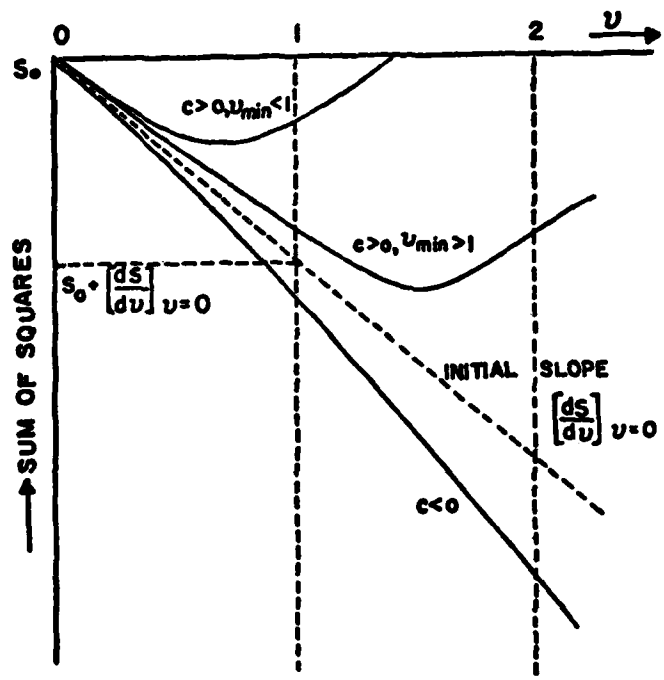

Figure 4. Various quadratic curves approximating the sum of squares along Gauss vector.

$$\hat{v} = \frac{(\underset{\sim}{\varepsilon}_o - \underset{\sim}{\varepsilon}_g)'\underset{\sim}{\varepsilon}_o}{(\underset{\sim}{\varepsilon}_o - \underset{\sim}{\varepsilon}_g)(\underset{\sim}{\varepsilon}_o - \underset{\sim}{\varepsilon}_g)}, \tag{6.7}$$

whence our estimate of parameters is obtained by $\underset{\sim}{\theta}^{(1)} = \underset{\sim}{\theta}^{(o)} + \hat{v}(\underset{\sim}{\theta}^{(g)} - \underset{\sim}{\theta}^{(o)})$. Again, computing $\hat{v}$ is very simple and makes use of information already available.[2]

In the sample space, modification B corresponds to dropping a perpendicular line from $\underset{\sim}{y}$ to $\underset{\sim}{f}_g - \underset{\sim}{f}_o$ whose foot gives the vector $(1 - \hat{v})\underset{\sim}{f}_o + \hat{v}\underset{\sim}{f}_g$. This is illustrated in Figure 5 for a one parameter model. The relationship of this procedure to modification A can be seen as follows. The sum of squares of the estimated residuals can be written as

$$\underset{\sim}{\varepsilon}'\underset{\sim}{\varepsilon} = (\underset{\sim}{y} - \underset{\sim}{f}_o - v(\underset{\sim}{f}_g - \underset{\sim}{f}_o))'(\underset{\sim}{y} - \underset{\sim}{f}_o - v(\underset{\sim}{f}_g - \underset{\sim}{f}_o)) \tag{6.8}$$

where $\underset{\sim}{f}_g$ is the $n \times 1$ vector of $f(\underset{\sim}{\xi}_u, \underset{\sim}{\theta}^{(g)})$, $u = 1,2,\ldots,n$. This is quadratic in v and passing through the points $(0,S_o)$ and $(1,S_g)$. Furthermore, the initial slope of the sum of squares of the estimated residuals is given by

$$\left[\frac{d\underset{\sim}{\varepsilon}'\underset{\sim}{\varepsilon}}{dv}\right]_{v=0} = -2(\underset{\sim}{f}_g - \underset{\sim}{f}_o)'(\underset{\sim}{y} - \underset{\sim}{f}_o) = -2(\underset{\sim}{f}_g - \underset{\sim}{f}_o)'\underset{\sim}{\varepsilon}_o \tag{6.9}$$

which is identical to the initial slope used in the previous method provided that $\underset{\sim}{f}_g = \underset{\sim}{f}_o + \underset{o}{X}(\underset{\sim}{\theta}^{(g)} - \underset{\sim}{\theta}^{(o)})$.

7. Example

In comparing various methods little in the way of general conclusions can be based on the performance of particular examples. The following simple example, taken from Box and Hunter [8] in an abbreviated form, is provided only for the purpose of gaining some preliminary ideas of the behavior of the procedures we have discussed.

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[2] When the criterion to stop the iterative process is made too stringent, in the extreme neighborhood of the minimum both the numerator and the denominator of (6.3) and (6.7) may become too small for the particular arithmetic precision being used. A precautionary provision that checks this is desirable to avoid unnecessary use of resources.

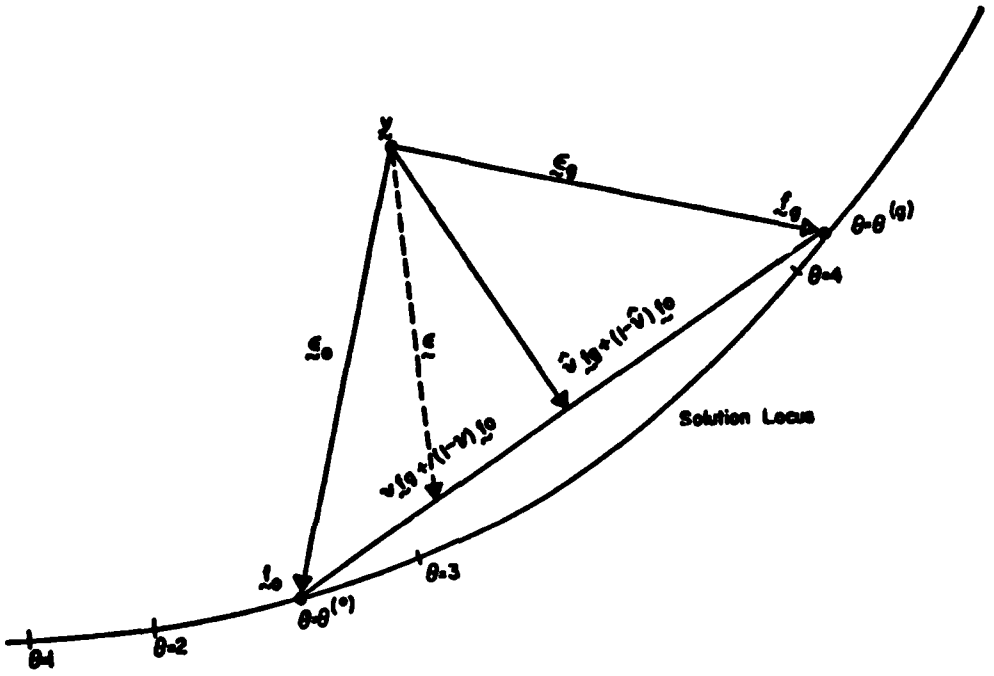

Figure 5. Sample space representation of modification B for the case of one parameter model.

The model is $f(\underset{\sim}{\xi},\underset{\sim}{\theta}) = \theta_1\theta_2\xi_1/(1 + \theta_1\xi_1 + 5000\xi_2)$ and the observations (ξ_1,ξ_2,y) are (1,1,0.1165), (2,1,0.2114), (1,2,0.0684) and (2,2,0.1159). The sum of squares surface, plotted in Figure 6, is very curved and ridgy. The values $(\theta_1,\theta_2) = (300,6)$ corresponding to P_o in the figure are the chosen initial estimates.

Figure 7 shows the result for five different methods. It shows the number of times, n_f, that $f(\underset{\sim}{\xi},\underset{\sim}{\theta})$ has to be evaluated before the iterative process reaches the point of minimum P_m (at which the sum of squares = 3.82750×10^{-5}). For the two methods that use the (λ,ν) algorithm n_f is shown for various choices of λ_o and ν, while that for the methods which do not depend on any control parameters is indicated by a horizontal line.

Considering that the methods with the (λ,ν) algorithm require a suitable choice of λ_o and ν in advance, the behavior of the modified Gauss methods with modifications A and B is certainly not discouraging. It will also be interesting that the modified Gauss method with the (λ,ν) algorithm appears stable over a wide range of λ_o, if we recall that the modified Gauss solution is the result of the constrained minimization in the space which requires no interpolation among the two classical approaches that often contradict each other.

8. Conclusion

The Levenberg-Marquardt's constrained iteration has been widely programmed and used. One apparent justification is that it provides a compromise between the steepest descent method and the Gauss method. However, if the parameters are transformed into the linearly invariant metric, the steepest descent vector and the Gauss solution vector are found to be identical and thus there is no need to compromise between directions given by these two vectors. It is also shown that the constrained minimization in the linearly invariant metric is equivalent to using in the original metric the modified Gauss method

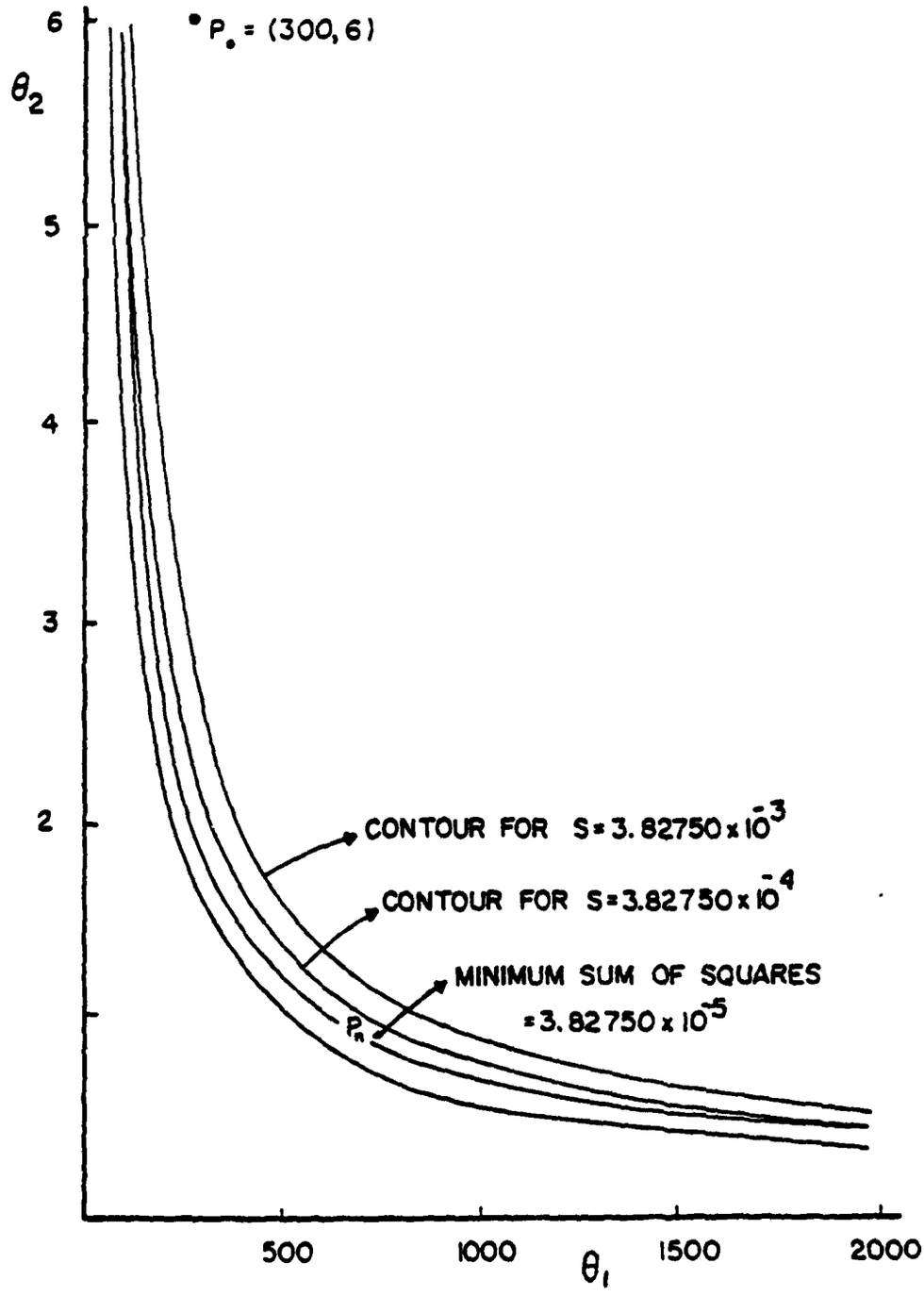

Figure 6. Sum of squares contours for the example.

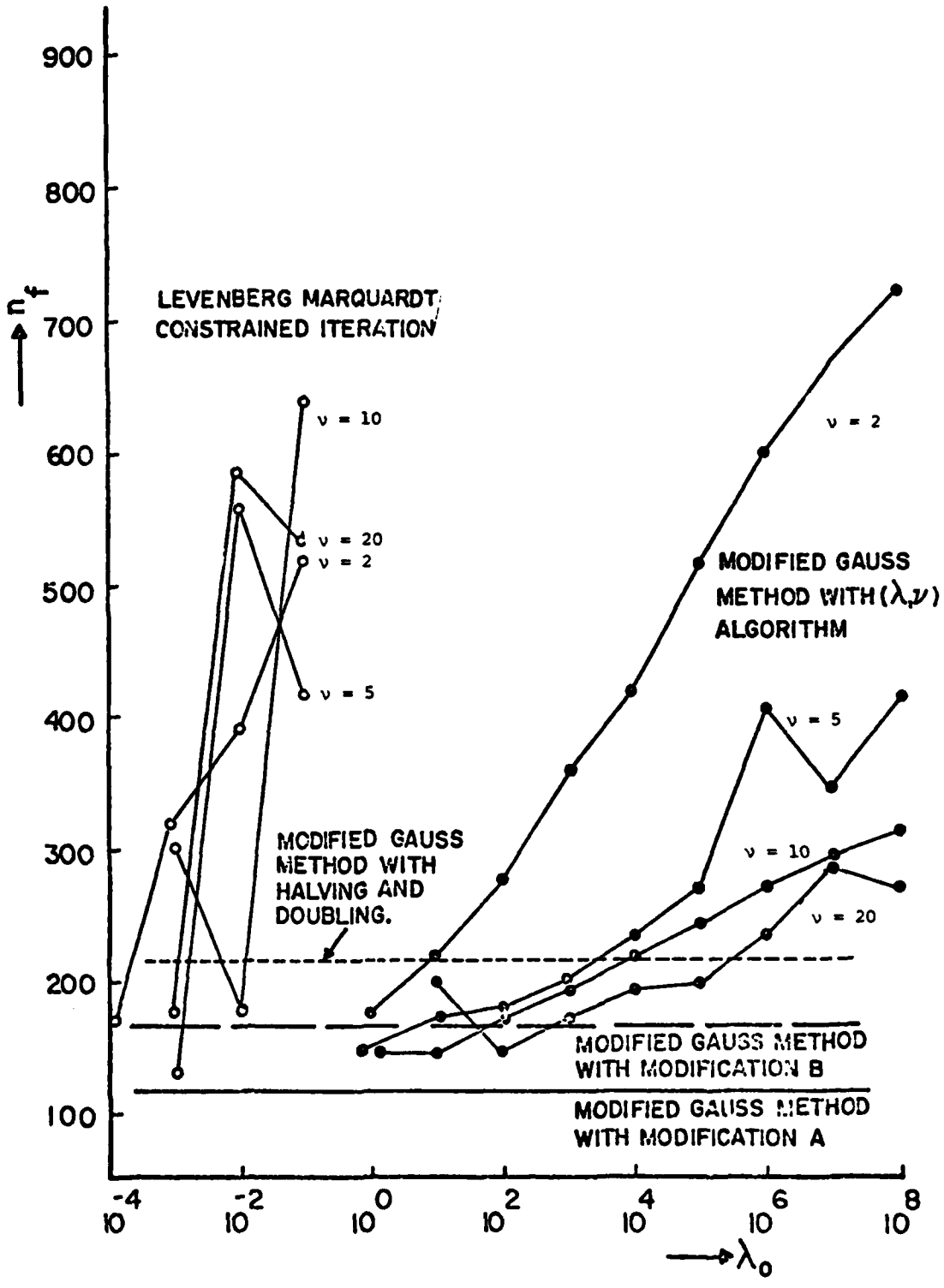

Figure 7. Comparison of five different procedures in the example.

which was proposed earlier. Two methods are proposed to determine how far one should go along the Gauss vector. These both have the virtue that their computation only involves information that already exists.

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Gauss suggested that, when the model is a nonlinear function of parameters, least squares parameter estimates might be obtained by iterative linearization. To prevent difficulties in convergence, Levenberg, and later Marquardt, proposed a constrained minimization procedure using a scale-invariant metric for the parameters. If, as seems sensible, the minimization is conducted in a metric which is also linearly invariant then the Levenberg-Marquardt method is equivalent to a simple modification of the Gauss iteration proposed earlier. Methods for deciding, at each stage, how far to move along the Gauss solution vector are introduced which make economic use of the available information.

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